Lecture outline

- Dimensionality reduction
  - SVD/PCA
  - CUR decompositions
- Nearest-neighbor search in low dimensions
  - kd-trees

Datasets in the form of matrices

We are given **n** objects and **d** features describing the objects. (Each object has **d** numeric values describing it.)

Dataset

An **n-by-d** matrix **A**, A_{ij} shows the "***importance***" of feature **j** for object **i**.

Every row of **A** represents an object.

Goal

1. **Understand** the structure of the data, e.g., the underlying process generating the data.
2. **Reduce the number of features** representing the data

Market basket matrices

d products
(e.g., milk, bread, wine, etc.)

n customers

$$\begin{pmatrix} \\ A \\ \\ \end{pmatrix}$$

$\mathbf{A_{ij}}$ = quantity of **j**-th product purchased by the **i**-th customer

Find a subset of the products that characterize customer behavior

Social-network matrices

$$
\begin{array}{cc}
 & \textbf{d}\text{ groups} \\
 & \text{(e.g., BU group, opera, etc.)} \\
\textbf{n}\text{ users} & \left(\begin{array}{c} \\ \\ A \\ \\ \end{array} \right)
\end{array}
$$

A_{ij} = partitiçipation of the **i**-th user in the **j**-th group

Find a subset of the groups that accurately clusters social-network users

Document matrices

$$
\begin{array}{cc}
 & \textbf{d}\ \text{terms} \\
 & \text{(e.g., theorem, proof, etc.)} \\
\textbf{n}\ \text{documents} & \left(\begin{array}{c} \\ A \\ \\ \end{array} \right)
\end{array}
$$

A_{ij} = frequency of the **j**-th term in the **i**-th document

Find a subset of the terms that accurately clusters the documents

Recommendation systems

$$\begin{array}{cc} & d \text{ products} \\ n \text{ customers} & \left(\begin{array}{c} A \\ A_{ij} = \text{frequency of the } j\text{-th product is bought by the } i\text{-th customer} \end{array} \right) \end{array}$$

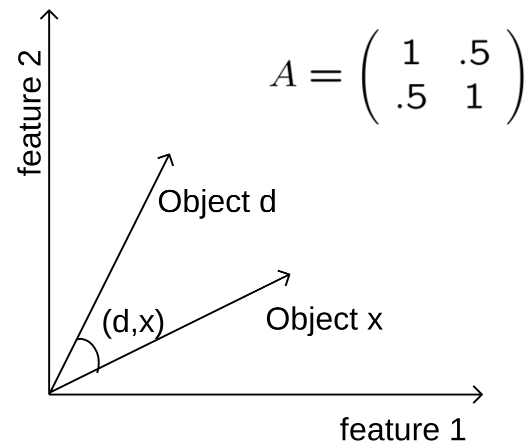
Find a subset of the products that accurately describe the behavior or the customers

The Singular Value Decomposition (SVD)

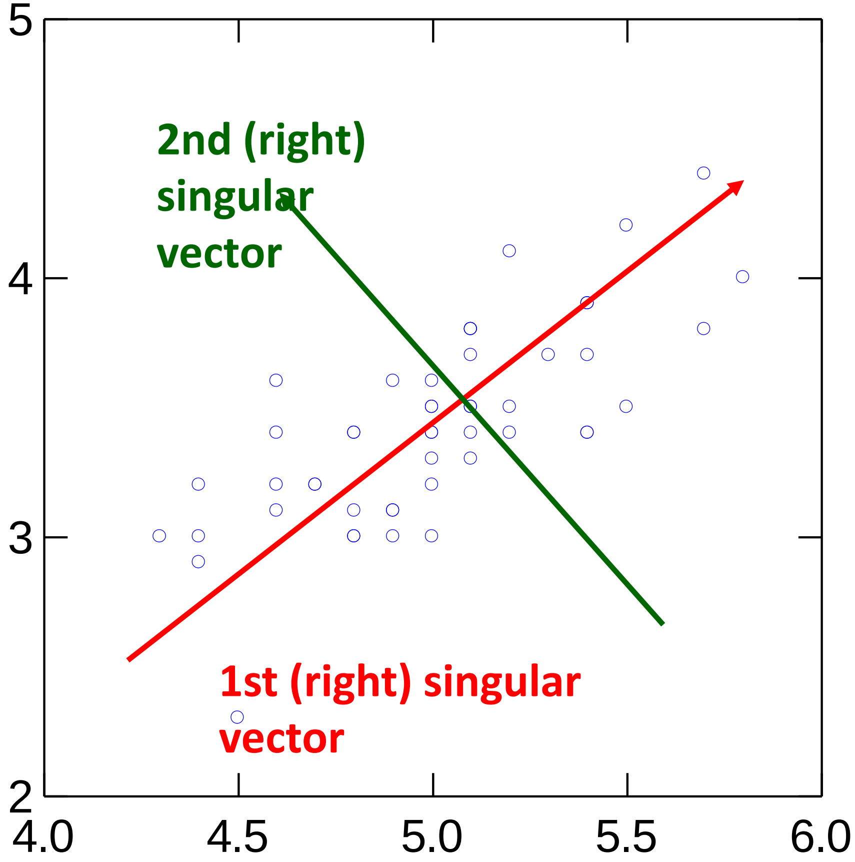
Data matrices have **n** rows (one for each object) and **d** columns (one for each feature).

<ins>Rows:</ins> vectors in a Euclidean space,

Two objects are "***close***" if the angle between their corresponding vectors is small.



SVD: Example



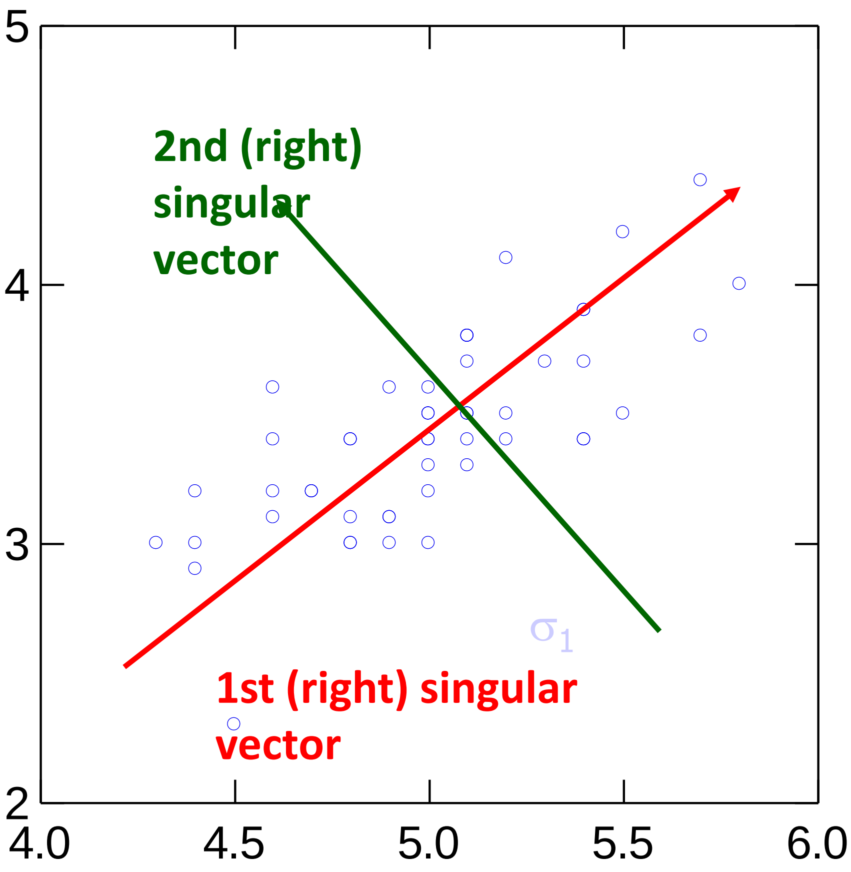
Input: **2-d** dimensional points

Output:

1st (right) singular vector:
direction of maximal variance,

2nd (right) singular vector:
direction of maximal variance, after removing the projection of the data along the first singular vector.

Singular values



σ_1: measures how much of the data variance is explained by the first singular vector.

σ_2: measures how much of the data variance is explained by the second singular vector.

SVD decomposition

$$\begin{pmatrix} \quad A \quad \end{pmatrix} = \begin{pmatrix} \quad U \quad \end{pmatrix} \cdot \begin{pmatrix} \Sigma \end{pmatrix} \cdot \begin{pmatrix} \quad V \quad \end{pmatrix}^T$$

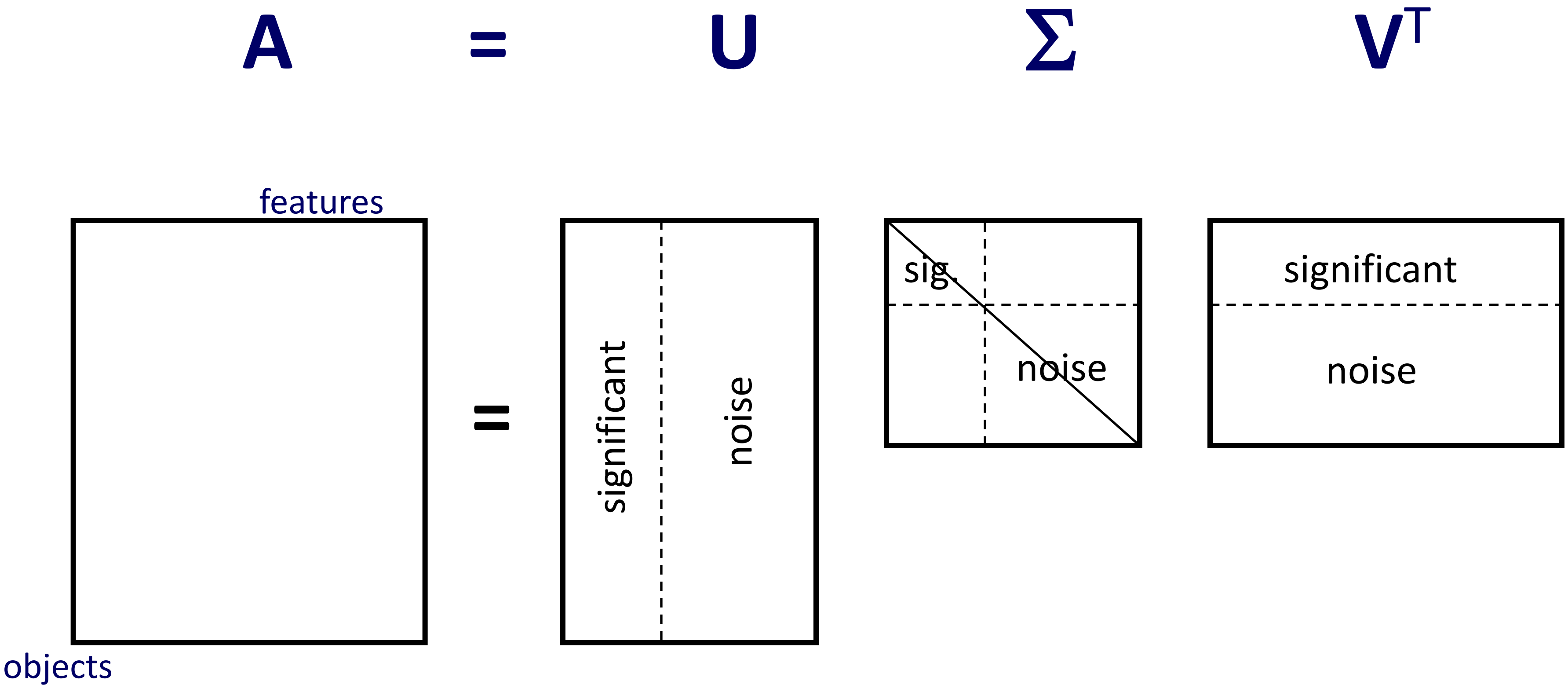
n x d **n x ℓ** **ℓ x ℓ** **ℓ x d**

U (V): orthogonal matrix containing the left (right) singular vectors of **A.**

Σ: diagonal matrix containing the **singular values** of **A:**
($\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_\ell$)

Exact computation of the SVD takes **O(min{mn², m²n})** time. The top *k* left/right singular vectors/values can be ***computed faster*** using Lanczos/Arnoldi methods.

SVD and Rank-k approximations



Rank-k approximations (A_k)

$$\underset{n \times d}{\begin{pmatrix} & & \\ & A_k & \\ & & \end{pmatrix}} = \underset{n \times k}{\begin{pmatrix} & & \\ & U_k & \\ & & \end{pmatrix}} \cdot \underset{k \times k}{\begin{pmatrix} & \Sigma_k & \end{pmatrix}} \cdot \underset{k \times d}{\begin{pmatrix} & V_k^T & \end{pmatrix}}$$

A_k is the **best** approximation of **A**

U_k (V_k): orthog

singular vecto

Σ_k: diagonal ma

A_k is an approximation of **A**

SVD as an optimization problem

Find **C** to minimize:

$$\min_{C} \left\| \underset{n\times d}{A} - \underset{n\times k}{C} \ \underset{k\times d}{X} \right\|_F^2$$

$$\|A\|_F^2 = \sum_{i,j} A_{ij}^2$$

Given **C** it is easy to find **X** from standard least squares. However, the fact that we can find the optimal **C** is fascinating!

PCA and SVD

- PCA is SVD done on **centered** data
- PCA looks for such a direction that the data projected to it has the maximal variance
- PCA/SVD continues by seeking the next direction that is orthogonal to all previously found directions
- All directions are orthogonal

How to compute the PCA

- Data matrix **A**, ***rows = data points***, ***columns = variables*** (attributes, features, parameters)

1. Center the data by subtracting the mean of each column
2. Compute the SVD of the centered matrix **A'** (i.e., find the first **k** singular values/vectors)
   $\mathbf{A' = U\Sigma V^T}$
3. The principal components are the columns of **V**, the coordinates of the data in the basis defined by the principal components are $\mathbf{U\Sigma}$

Singular values tell us something about the variance

- The variance in the direction of the **k**-th principal component is given by the corresponding singular value $\boldsymbol{\sigma_k^2}$

- Singular values can be used to estimate how many components to keep

- ***Rule of thumb:*** keep enough to explain ***85%*** of the variation:

$$\frac{\sum_{j=1}^{k} \sigma_j^2}{\sum_{j=1}^{n} \sigma_j^2} \approx 0.85$$

SVD is **the Rolls-Royce and the Swiss Army Knife of Numerical Linear Algebra.”***

*Dianne O’Leary, MMDS ’06

SVD as an optimization problem

Find **C** to minimize:

$$\min_C \left\| \underset{n\times d}{A} - \underset{n\times k}{C}\ \underset{k\times d}{X} \right\|_F^2$$

$$\|A\|_F^2 = \sum_{i,j} A_{ij}^2$$

Given **C** it is easy to find **X** from standard least squares. However, the fact that we can find the optimal **C** is fascinating!

The **CX**-decomposition

Find **C** **that contains subset of the columns of A** to minimize:

$$\min_C \left\| \underset{n\times d}{A} - \underset{n\times k}{C}\ \underset{k\times d}{X} \right\|_F^2$$

$$\|A\|_F^2 = \sum_{i,j} A_{ij}^2$$

Given **C**it is easy to find **X** from standard least squares.
However, finding **C** is now hard!!!

Why CX-decomposition

- If **A** is an object-feature matrix, then selecting **“representative” columns** is equivalent to selecting **“representative” features**

- This leads to easier ***interpretability***; compare to eigenfeatures, which are linear combinations of all features.

Algorithms for the **CX** decomposition

- The **SVD-based** algorithm

- The **greedy** algorithm

- The **k-means-based** algorithm

Algorithms for the **CX** decomposition

- The **SVD-based** algorithm
  - Do SVD first
  - Map **k** columns of **A** to the left singular vectors
- The **greedy** algorithm
  - Greedily pick **k** columns of **A** that minimize the error
- The **k-means-based** algorithm
  - Find **k** centers (by clustering the columns)
  - Map the **k** centers to columns of **A**

Discussion on the CX decomposition

- The vectors in **C** are not orthogonal – they do not define a space
- It maintains the sparcity of the data

Nearest Neighbour in low dimensions

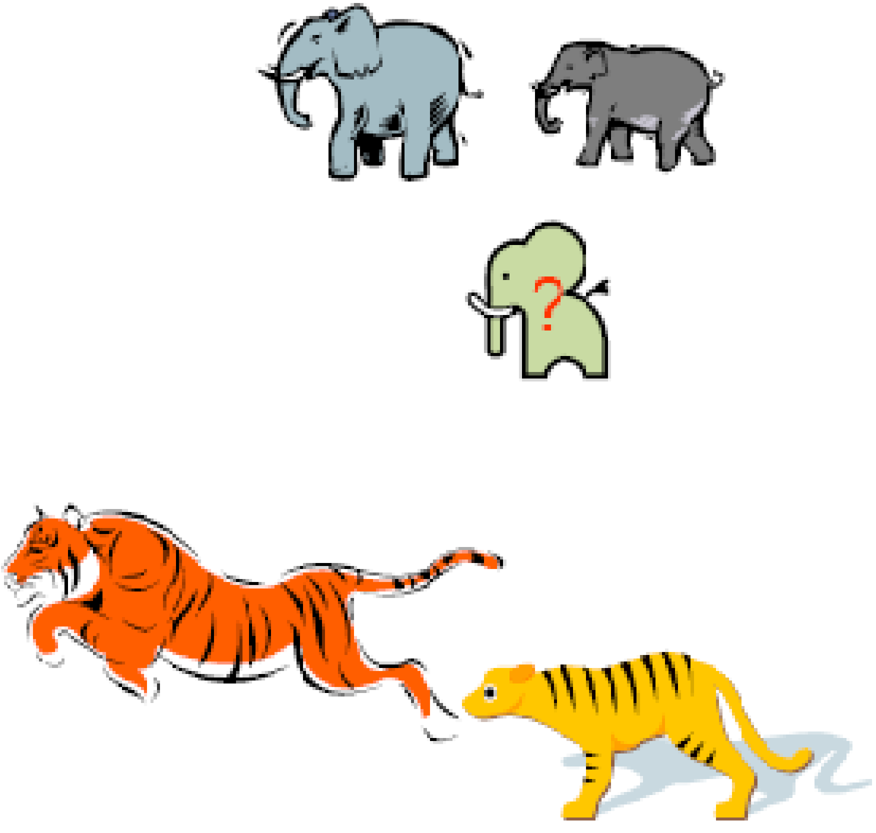
Definition

- Given: a set **X** of **n** points in **R^d**
- Nearest neighbor: for any query point **$q \in R^d$** return the point **$x \in X$** minimizing **$L_p(x,q)$**

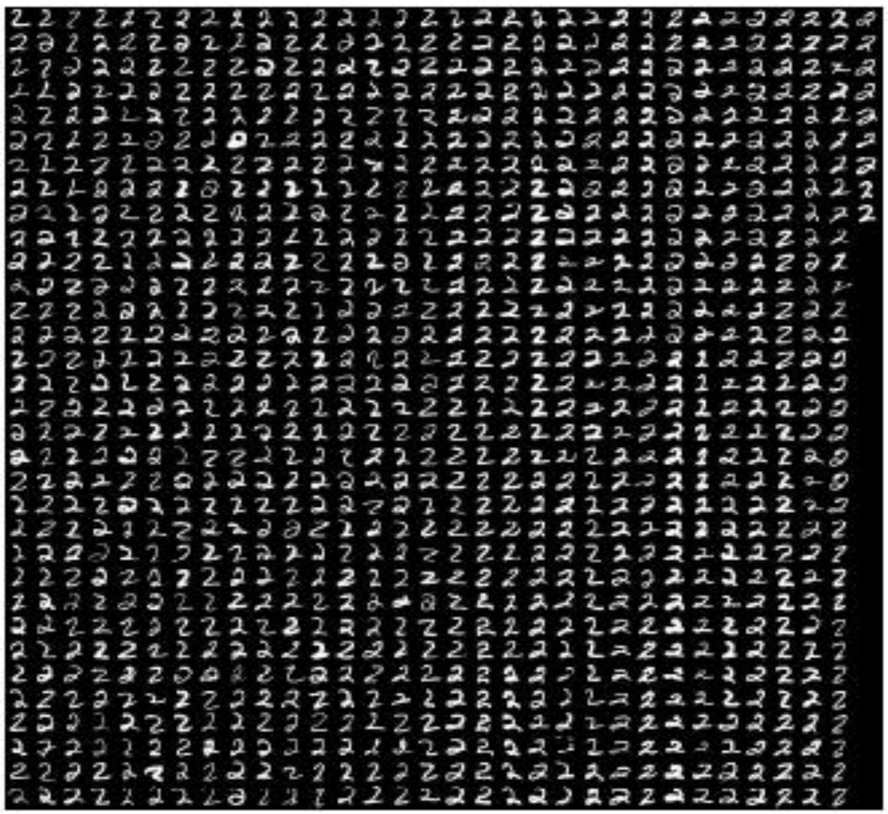
Motivation

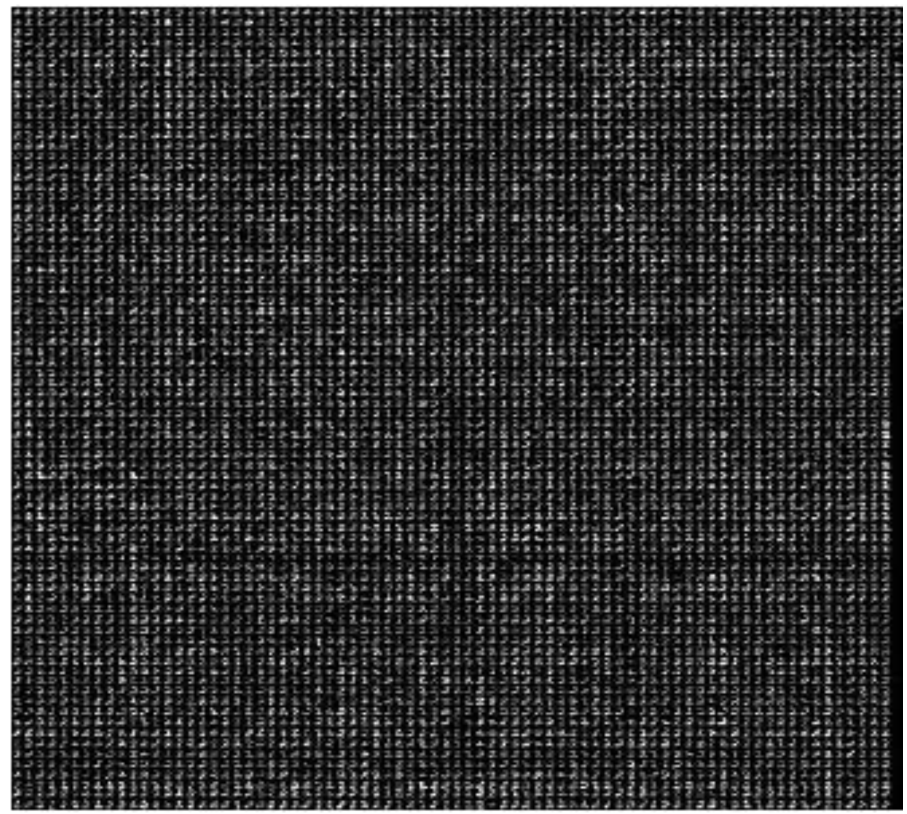
- **Learning:** Nearest neighbor rule
- **Databases:** Retrieval
- Donald Knuth in vol.3 of ***The Art of Computer Programming*** called it the post-office problem, referring to the application of assigning a resident to the ***nearest-post office***

Nearest neighbor rule



MNIST dataset “2”





Methods for computing NN

- **Linear scan: O(nd)** time

- This is pretty much all what is known for exact algorithms with theoretical guarantees

- In practice:
  - ***kd-trees*** work “well” in “low-medium” dimensions

2-dimensional kd-trees

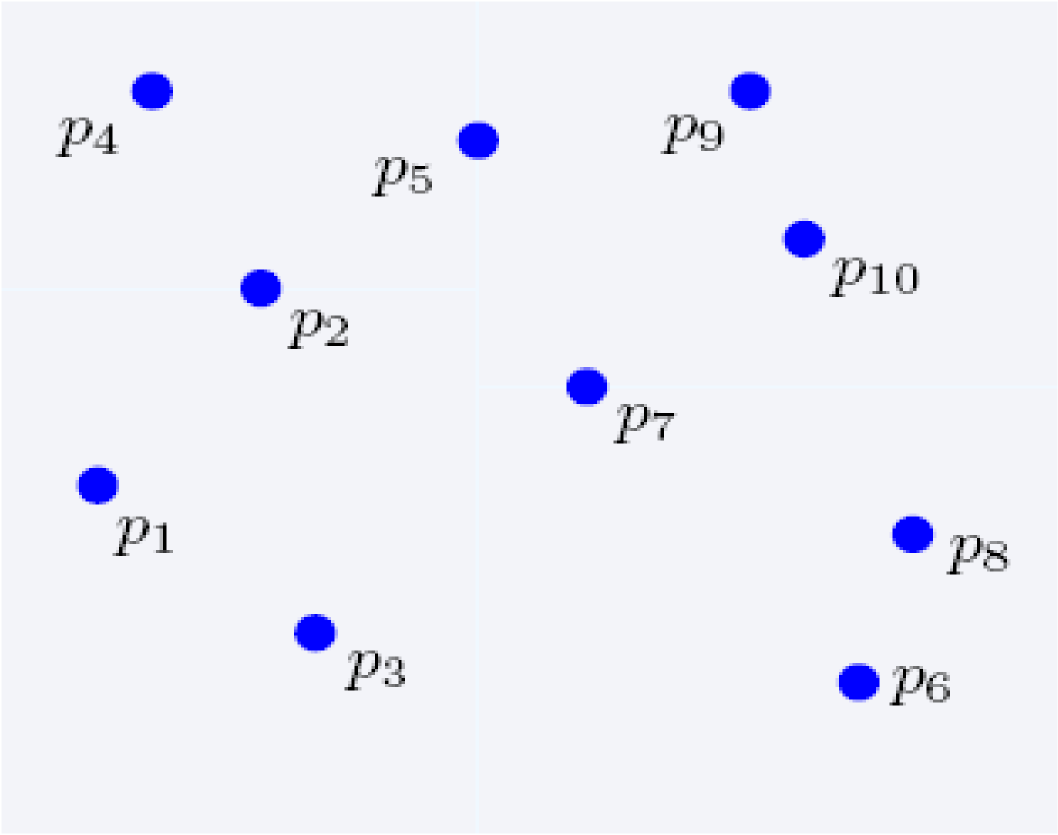
- A data structure to support range queries in $\mathbf{R^2}$
  - Not the most efficient solution in theory
  - Everyone uses it in practice

- Preprocessing time: $O(n\log n)$
- Space complexity: $O(n)$
- Query time: $O(n^{1/2}+k)$

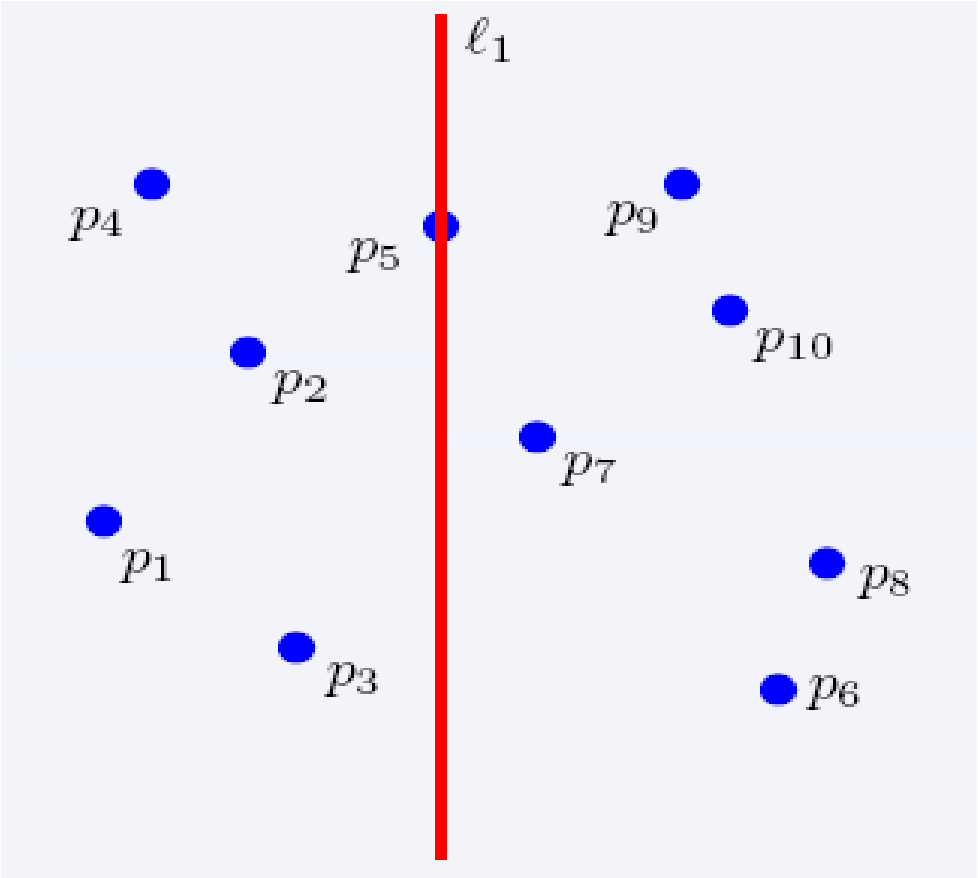
2-dimensional kd-trees

- Algorithm:
  - Choose **x** or **y** coordinate (alternate)
  - Choose the median of the coordinate; this defines a horizontal or vertical line
  - Recurse on both sides
- We get a binary tree:
  - Size **O(n)**
  - Depth **O(logn)**
  - Construction time **O(nlogn)**

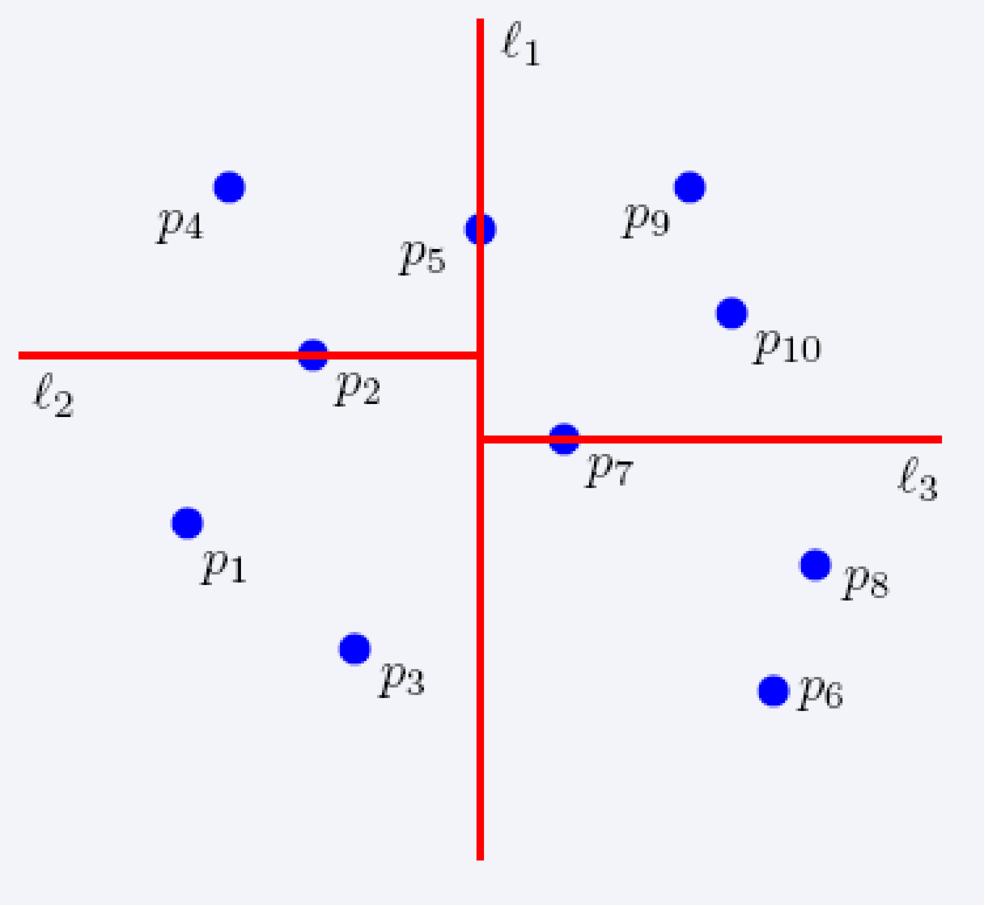
Construction of kd-trees



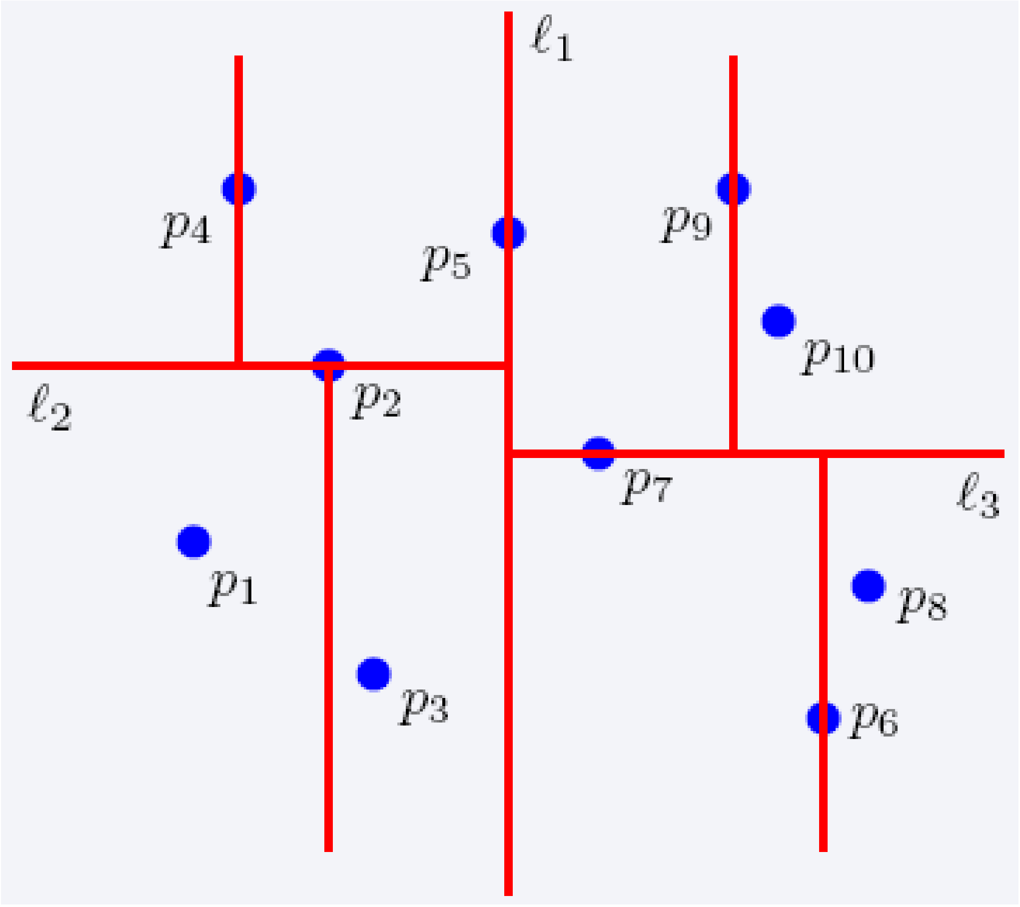
Construction of kd-trees



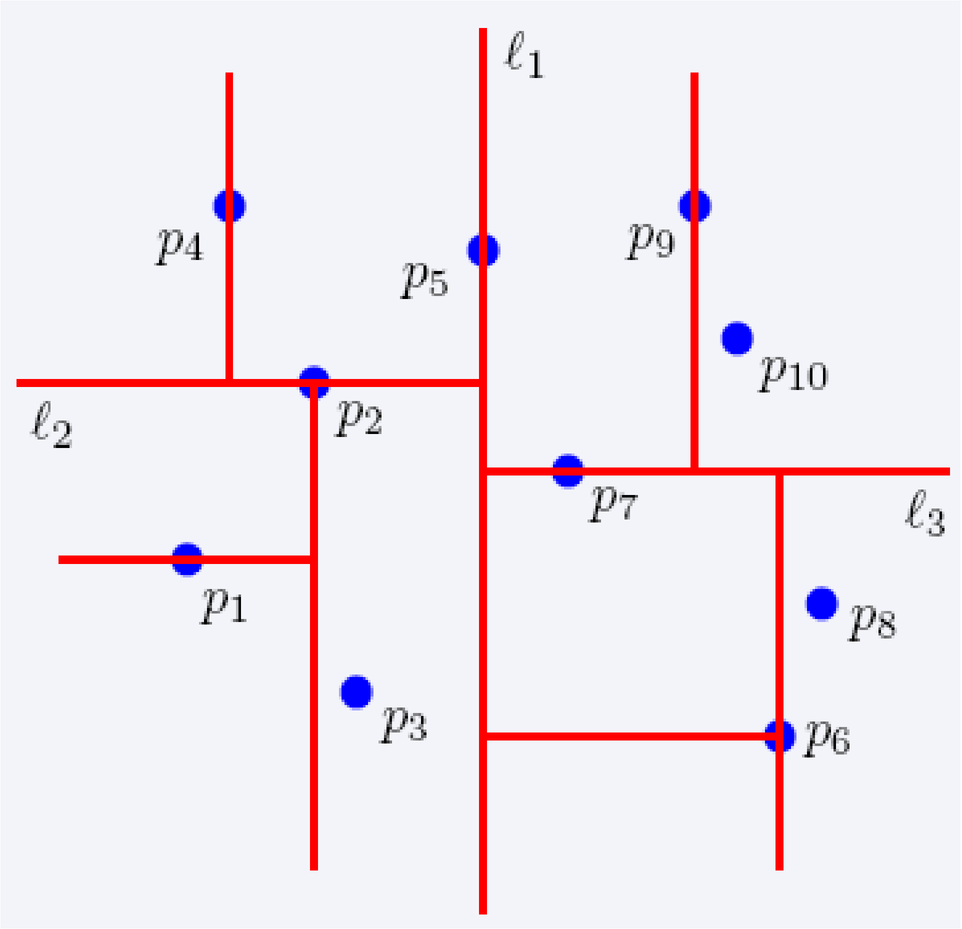
Construction of kd-trees



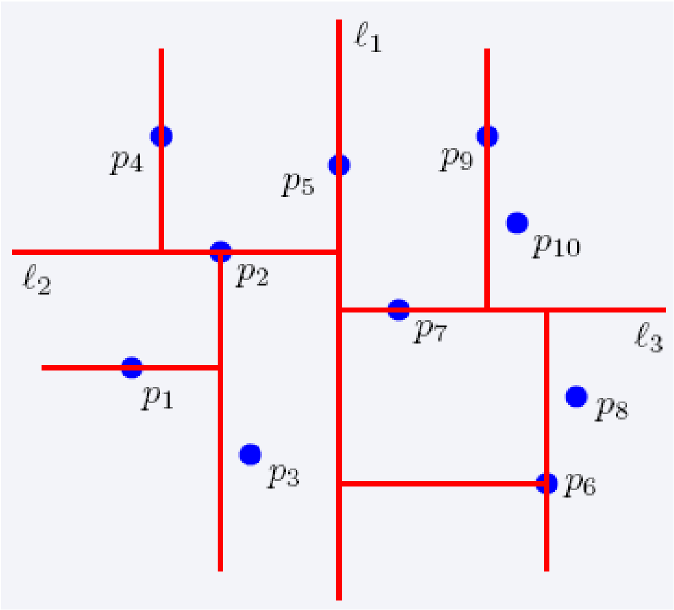
Construction of kd-trees

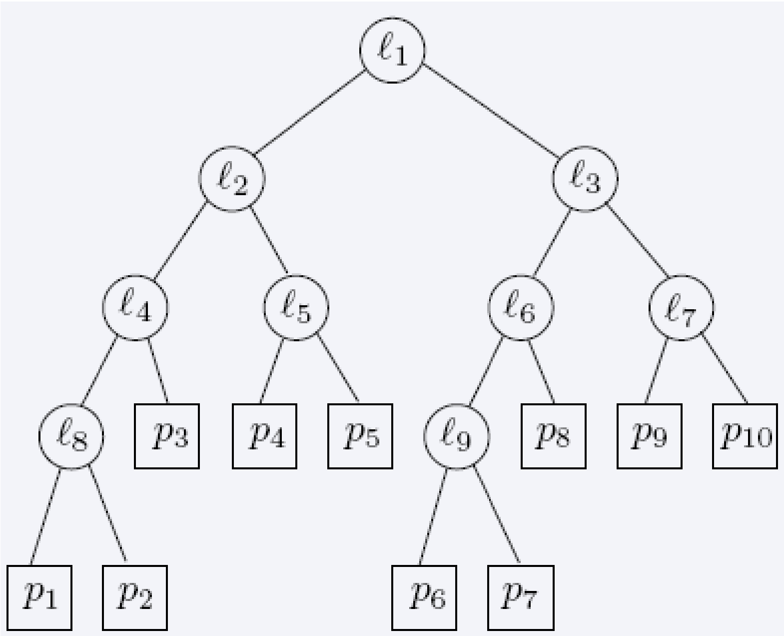


Construction of kd-trees

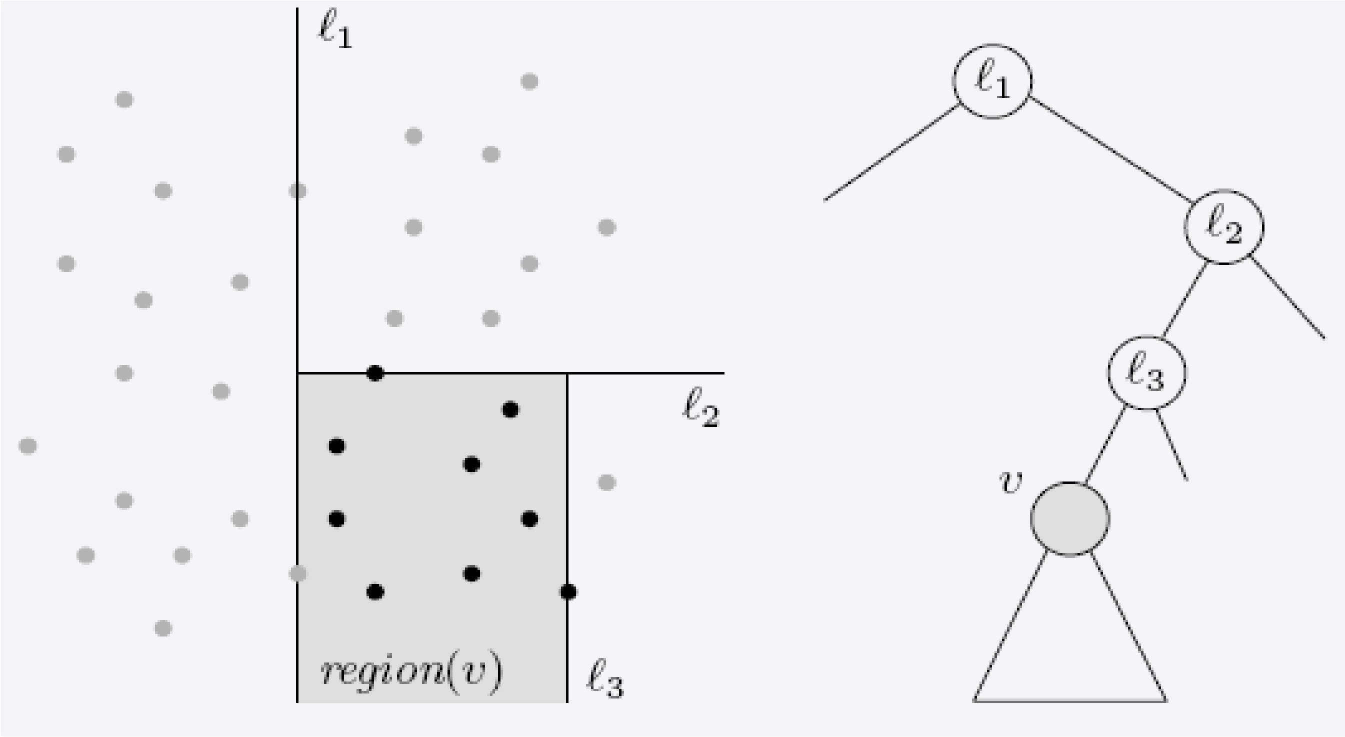


The complete kd-tree





Region of node **v**



Region(v) : the subtree rooted at v stores the points in black dots

Searching in kd-trees

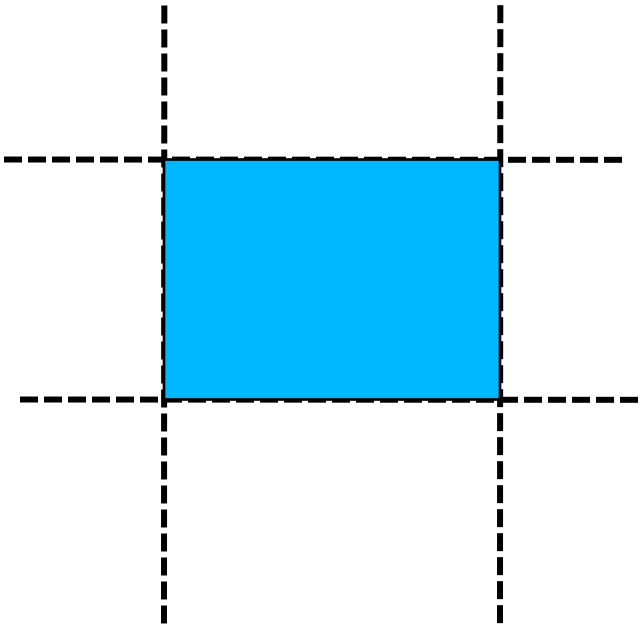
- Range-searching in **2-d**
  - Given a set of **n** points, build a data structure that for any query rectangle **R** reports all point in **R**

kd-tree: range queries

- Recursive procedure starting from **v = root**
- **Search (v,R)**
  - If **v** is a leaf, then report the point stored in **v** if it lies in **R**
  - Otherwise, if **Reg(v)** is contained in **R**, report all points in the **subtree(v)**
  - Otherwise:
    - If **Reg(left(v))** intersects **R**, then **Search(left(v),R)**
    - If **Reg(right(v))** intersects **R**, then **Search(right(v),R)**

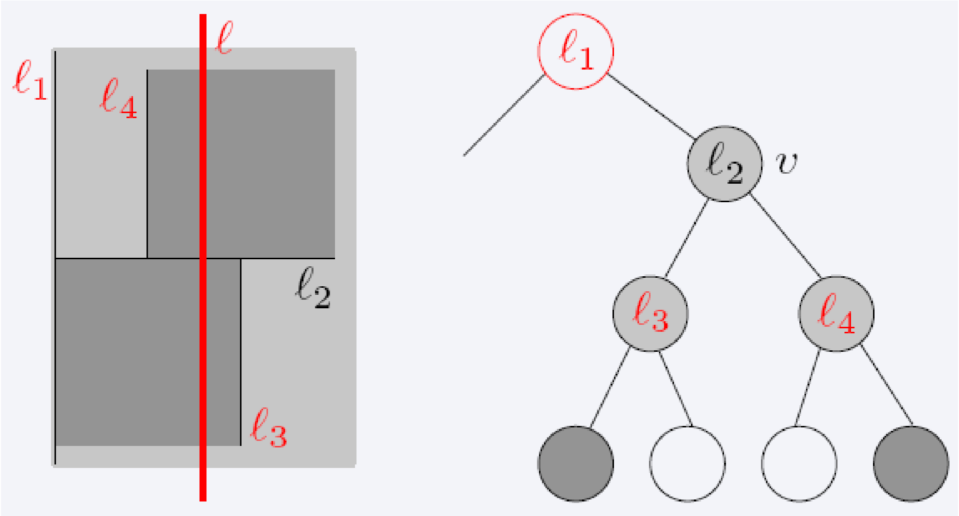
Query time analysis

- We will show that **Search** takes at most **$O(n^{1/2}+P)$** time, where **P** is the number of reported points
  - The total time needed to report all points in all sub-trees is **$O(P)$**
  - We just need to bound the number of nodes **v** such that **region(v)** intersects **R** but is not contained in **R** (i.e., boundary of R intersects the boundary of **region(v)**)
  - ***gross overestimation***: bound the number of **region(v)** which are crossed by any of the **4** horizontal/vertical lines



Query time (Cont'd)

- **Q(n):** max number of regions in an n-point kd-tree intersecting a (say, vertical) line?



- If **ℓ** intersects **region(v)** (due to vertical line splitting), then after two levels it intersects **2** regions (due to 2 vertical splitting lines)
- The number of regions intersecting **ℓ** is **Q(n)=2+2Q(n/4)** → **Q(n)=(n$^{1/2}$)**

d-dimensional kd-trees

- A data structure to support range queries in $\mathbf{R}^d$

- Preprocessing time: $\mathbf{O(n\log n)}$
- Space complexity: $\mathbf{O(n)}$
- Query time: $\mathbf{O(n^{1-1/d}+k)}$

Construction of the **d**-dimensional kd-trees

- The construction algorithm is similar as in **2-d**
- At the root we split the set of points into two subsets of same size by a hyperplane vertical to $\mathbf{x_1}$-axis
- At the children of the root, the partition is based on the second coordinate: $\mathbf{x_2}$-coordinate
- At depth **d**, we start all over again by partitioning on the first coordinate
- The recursion stops until there is only one point left, which is stored as a leaf